

# Superconductivity and antiferromagnetism in a hard-core boson spin-1 model in two dimensions

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A model of hard-core bosons and spin-1 sites with single-ion anisotropy is proposed to approximately describe hole pairs moving in a background of singlets and triplets with the aim of exploring the relationship between superconductivity and antiferromagnetism. The properties of this model at zero temperature were investigated using quantum Monte Carlo techniques. The most important feature found is the suppression of superconductivity, as long range coherence of preformed pairs, due to the presence of both antiferromagnetism and  $S^z = \pm 1$  excitations. Indications of charge ordered and other phases are also discussed.

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The mechanism of pairing and the establishment of long-range superconducting (SC) coherence are still central issues in the theory of high- $T_c$  superconductivity.<sup>1</sup> Although strong electronic correlations are the essential component of most proposed scenarios for the SC phase and its nearby antiferromagnetic (AF) Mott insulating phase, important experimental results such as the resonant peak<sup>2</sup> have not been satisfactorily explained by such scenarios. Part of the theoretical limitations are related to the enormous difficulty in studying a microscopic model like the  $t$ - $J$  model, which is the simplest model that describes the dynamics of holes in an AF background. From the numerical point of view, the main difficulty consists in reaching large enough clusters. This problem is really critical in the presence of inhomogeneities, like the well-known stripes<sup>3</sup> and the ones that have more recently become the center of intensive research.<sup>4</sup>

In this article, we propose and analyze a highly simplified effective Hamiltonian in two dimensions (2D) to study the interplay between superconductivity and antiferromagnetism. Our goal is to describe the movement of boson hole pairs in a sea of magnetic excitations. This model implies a reduction in the Hilbert space with respect to the  $t$ - $J$  model, which is convenient for exact diagonalization calculations, and the elimination of the “minus sign” problem<sup>5</sup> which severely inhibits the application of quantum Monte Carlo (QMC) techniques to fermions in 2D. Such a model could be useful to study experimental features like the ones mentioned earlier and inhomogeneous states in which there are phase separated SC and AF regions.

Although I shall not attempt a derivation of the present model from a more microscopic one like the  $t$ - $J$  model, I shall present some heuristic arguments to guide the physical interpretation of the results obtained and shown below. Let us start with the  $t$ - $J$  model on the square lattice. A coarse-grained Hamiltonian can be obtained by mapping two nearest neighbor (NN) sites (a “dimer”) of the original lattice onto a site of the effective lattice.<sup>6</sup> Due

to the constraint of no double-occupancy in the starting model, there are nine states in each of the coarse-grained sites. Since our purpose is to study the interplay between pairs and magnetic excitations, the states corresponding to only one hole in the original dimers are eliminated. Hence, we are left with five states per site which correspond to a singlet ( $S = 0$ ), a triplet ( $S = 1$ , and  $S^z = -1, 0, +1$ ), and a hole pair. Finally, the singlets play the role of the vacuum, and the hole pairs are described by bosons.<sup>7</sup> All these states are by construction hard-core entities. Of course, this coarse-graining procedure here outlined has been employed many times, particularly in the context of resonant valence bond (RVB) theories. By restoring the interactions between dimers, it has been shown<sup>8</sup> that the long-range AF order is recovered in the undoped case.

The physical underlying scenario is then one in which hole pairs move in a “soup” of singlets and triplets. The same states per site can be also found in “projected” SO(5) models<sup>9,10</sup> but in these models the interactions between them are essentially dictated by symmetry requirements rather than by microscopical considerations (see Fig. 1 below). An extreme case with no triplet excitations, i.e., a model of pairs as hard-core bosons, has been extensively considered to describe superfluid phases.<sup>11–13</sup>

However, the model studied in the present work contains a further simplification and hence it should be considered as a “toy model” of that scenario of pairs moving in a singlet-triplet soup. This simplification consists in considering doublets instead of triplets. This is achieved by assuming that all sites are occupied by triplets and pairs, and by adding to the Hamiltonian a single-ion anisotropy term (third term in Eq. (1) below) with a coupling constant  $\Lambda$ . For  $\Lambda \neq 0$ , the triplet states split into  $S^z = \pm 1$  doublets and  $S^z = 0$  singlets. Of course, the total spin is no longer a good quantum number. Let us introduce  $D = \sum_i (S_i^z)^2$ , the number of doublets. For  $\Lambda = 0$  there are only triplets in the model and then  $D$  goes to 2/3 of the number of triplets. For  $\Lambda \rightarrow \infty$  there are only singlets and then  $D \rightarrow 0$ . Assuming that

this quantity  $D$  evolves continuously between both limits then one could consider it as the analog, in this simplified model, of the number of triplet excitations in the singlet-triplet soup earlier discussed. In this sense, the single-ion anisotropy  $\Lambda$  would correspond to the chemical potential in the related SO(5) models.

The exchange interactions included in our model are those resulting from a single exchange in the original spin-1/2  $t$ - $J$  model, as shown in Fig. 1. The exchange interaction shown in Fig. 1(b) is not included in the projected SO(5) Hamiltonian. On the other hand, in that Hamiltonian, there is a term corresponding to the one shown in Fig. 1(c). However, this interaction has no microscopic origin in a  $t$ - $J$  like model because it does not conserve the total  $S^z$  and hence it is not included in our Hamiltonian. Then, the effective Hamiltonian here proposed is:<sup>14</sup>

$$\mathcal{H} = -t \sum_{\langle i,j \rangle, s} (b_{j,s}^\dagger c_{j,s} c_{i,s}^\dagger b_i + h.c.) + J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + \Lambda \sum_i (S_i^z)^2 + V \sum_{\langle i,j \rangle} n_i n_j \quad (1)$$

where  $c_{j,s}, c_{j,s}^\dagger$  are annihilation and creation operators of  $s = S^z = 0, \pm 1$  spins,  $b_i, b_i^\dagger$  are annihilation and creation operators of hole pairs,  $n_i = b_i^\dagger b_i$ . The exchange term is just the spin-1 Heisenberg term, and it captures the corresponding interactions shown in Fig. 1 in a simple way.

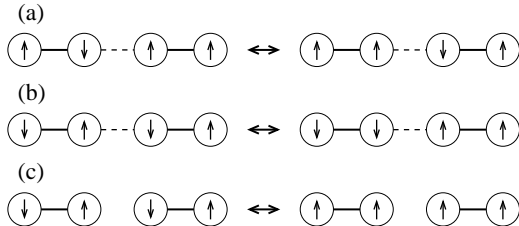


FIG. 1. Microscopic origin of exchange interactions. Dimers are indicated with bold lines. The exchange interaction between electrons in different dimers are shown with dashed lines. In terms of the total  $S^z$  of each dimer, case (a) corresponds to  $(0, +1) \leftrightarrow (+1, 0)$ , and (b) to  $(0, 0) \leftrightarrow (-1, +1)$ . The change (c),  $(0, 0) \leftrightarrow (+1, +1)$  has no microscopical origin.

The hopping term between pairs and doublets ( $s = \pm 1$  in the first term of Eq. (1)) induces the minus sign problem in the quantum Monte Carlo simulations and hence we shall not include it in most of the following study. The analogous term of hopping between pairs and triplets are also not included in the projected SO(5) Hamiltonian. Preliminary results obtained including this term show essentially the same qualitative features shown below for the parameters considered. Although in principle  $\Lambda$  should be determined by the internal dynamics of the

original  $t$ - $J$  model, in our effective model this is a parameter which we vary freely, in the same way as the spin chemical potential in the projected SO(5) model. Finally, our model contains a nearest neighbor Coulomb repulsion between pairs, to prevent phase separation in the low density region.<sup>10</sup>

We adopt  $t$  as the unit of energy. From previous studies of the hard-core boson model we adopt  $V = 3$ . It is not simple to determine a priori the ratio  $J/t$ .  $J$  should be of the order of the exchange coupling constant of the original Hamiltonian, although in some cases it may involve longer than NN interactions.  $t \sim t_0 t'_0 / \Delta_b$  where  $t_0$  ( $t'_0$ ) is the NN (longer than NN) hopping amplitude in the original  $t$ - $J$  model, and  $\Delta_b$  the cost of breaking a hole pair in the intermediate state. This ratio could be determined eventually a posteriori by e.g. matching the energies of small clusters of the original and the effective model. In the present work, we adopted a reasonably small value  $J/t = 0.3$ . We expect that the effect of a different value would just amount to quantitative shifting the phase boundaries without introducing qualitative new features. Of course, a more exhaustive parameter study should be done in the future.

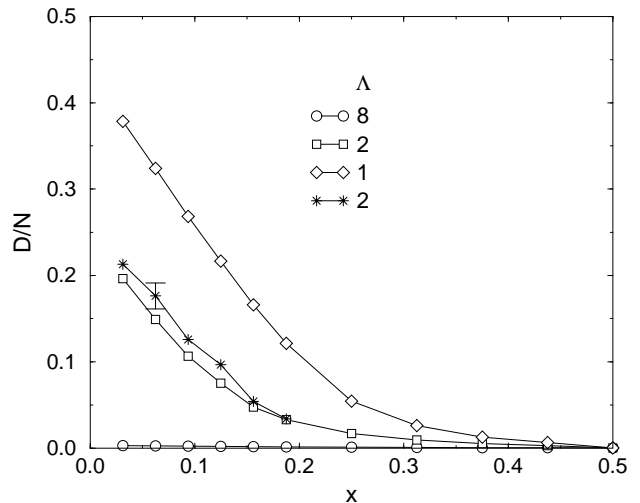


FIG. 2. Relative number of sites with  $S^z = \pm 1$  for various values of the single-ion anisotropy  $\Lambda$ . The stars correspond to the full Hamiltonian Eq. (1) at  $T = 0.2$  (in this case a typical error bar is shown).

All results shown below, except otherwise stated, correspond to the model Eq. (1) excluding  $s = \pm 1$  in the hopping term, and they were obtained by QMC techniques (conventional world-line algorithm) on the  $8 \times 8$  cluster with periodic boundary conditions. The temperature  $T$  was varied between  $0.2t$  and  $0.1t$ , i.e., considerably below the Kosterlitz-Thouless temperatures separating normal and SC phases found in previous studies on related models.<sup>13,10</sup> The Trotter number was kept at a standard value,  $\Delta\tau = 0.1$ . The results were finally extrapolated to zero temperature with an exponential law.

The error bars are about or smaller than the size of the symbols used, except otherwise stated.

The dependence of  $D/N$  ( $N$ : number of sites of the cluster), i.e. the relative number of  $S^z = \pm 1$  sites is shown in Fig. 2 as a function of the pair density  $x$  and for various values of  $\Lambda \geq 1$ . For  $\Lambda = 8$ ,  $D$  is negligible and hence this value of  $\Lambda$  is essentially the  $\Lambda \rightarrow \infty$  limit, i.e., hard-core pairs moving in a vacuum played by the singlets.<sup>11–13</sup> The continuity of  $D$  as  $\Lambda$  is increased from zero, at a fixed  $x$  is not a trivial problem. It is obvious that for  $J = 0$  there are no terms in the Hamiltonian to compensate the cost of the single-ion anisotropy term and hence there is a discontinuity in  $D$  as soon as  $\Lambda$  takes a nonzero value. The possibility of a finite critical value of  $J$ ,  $J_{cr}(x)$ , below which  $D$  is discontinuous with  $\Lambda$  will not be examined in the present work. It should also be noticed that, after dropping the  $s = \pm 1$  contributions to the first term of Eq. (1), another source of anisotropy appears between the  $S^z = 0, \pm 1$  components. This is reflected in  $D$  as it can be seen in Fig. 2 for  $\Lambda = 2$ .

In order to determine partially the phase diagram of this model in the  $\Lambda - x$  space, we compute the following quantities. In the first place, charge and spin correlations,  $C(\mathbf{r}) = \langle n_0 n_{\mathbf{r}} \rangle$ ,  $S(\mathbf{r}) = \langle S_0^z S_{\mathbf{r}}^z \rangle$ , respectively, together with their Fourier transforms  $C(\mathbf{k})$  and  $S(\mathbf{k})$ , i.e., the charge and spin static structure factors. In addition, we compute also the staggered correlations, i.e., including a factor  $(-1)^{x+y}$  in the sums of the previous expressions.

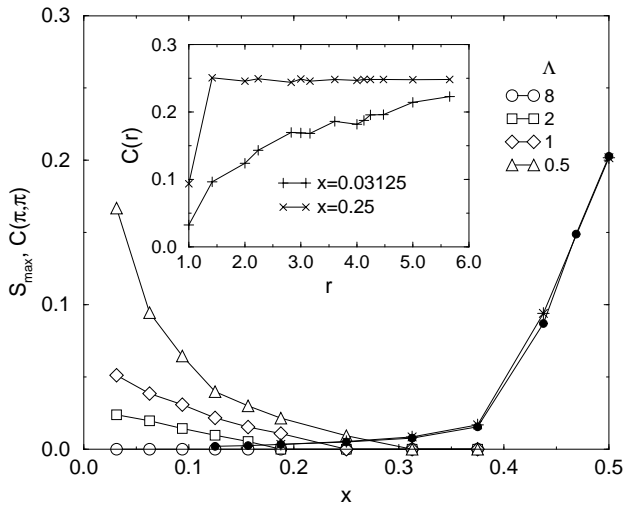


FIG. 3. Staggered spin correlations at the maximum distance (open symbols) as a function of pair density and for various values of  $\Lambda$ . The charge structure factor at  $(\pi, \pi)$  is shown for  $\Lambda = 8$  (circles) and  $\Lambda = 1$  (stars). In the inset, the charge correlations vs. distance are shown for  $\Lambda = 1$  at  $x = 0.03125$  (multiplied by 10) and  $x = 0.25$ .

In Fig. 3, the staggered spin correlations at the maximum distance  $r$ , are shown as a function of pair density and for several values of  $\Lambda$ . They indicate strong AF

correlations as  $\Lambda \rightarrow 0$ , particularly as  $x \rightarrow 0$ . i.e. as the pure spin-1 Heisenberg model is approached. The determination of the long-range character and of the boundary of the AF region as a function of  $\Lambda$  would imply a finite size scaling, which is out of the scope of the present study. The charge structure factor has a peak at  $(\pi, \pi)$  for all the parameter space  $(x, \Lambda)$  examined except at low densities. As shown in the Fig. 3, this structure factor is very weakly dependent with  $\Lambda$ , and hence the so-called “checkerboard solid” phase found in the hard-core boson limit<sup>11</sup> might extend down to  $\Lambda = 0$  at  $x \approx 0$  (see discussion below).

For pair densities lower than  $\approx 0.15$  and for  $\Lambda \approx 0$  we have detected indications of incommensurate charge ordering with  $q_{IC} = (\pi - \delta, \pi - \delta)$  below  $x = 0.06$ , and  $q_{IC} = (\pi - \delta, \pi)$  (and symmetry related points) above it, with  $\delta$  varying with pair density. In these cases, the charge structure factor is more than two orders of magnitude smaller than for  $(\pi, \pi)$  at  $x = 0.5$ .

In Fig. 4(a) the total energy per site vs. pair density for various  $\Lambda$  is shown. The region  $x \geq 0.4$  apparently presents a negative curvature which corresponds to phase separation (PS), although probably larger clusters would be needed to confirm this result. In this region, PS was found for  $\Lambda \rightarrow \infty$ ,  $0.39 \leq x \leq 0.5$  in the bulk limit using alternative criteria.<sup>13</sup>

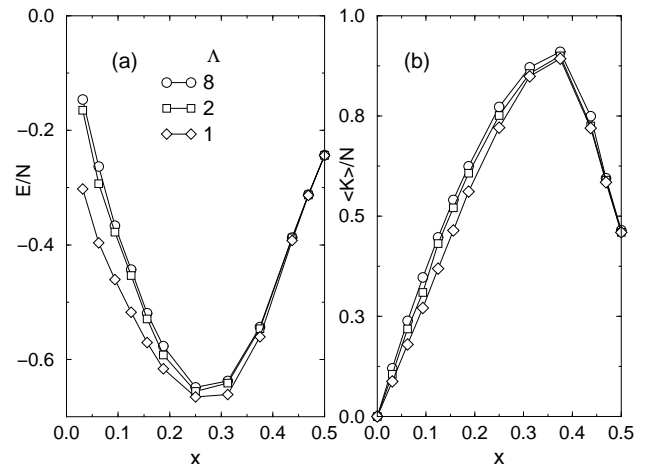


FIG. 4. (a) Energy per site, and (b) kinetic energy per site as a function of pair density and for several values of  $\Lambda$ .

Consistently with this indication of PS, pair-pair correlations (inset of Fig. 3) show a tendency of the holes to be at short distances as the density increases. This tendency is superimposed to a strong alternation corresponding to the peak in the charge structure factor at  $(\pi, \pi)$ . The second most important peaks correspond to  $q_{IC} = (\pi - \delta, \pi)$ ,  $\delta = \pi/4$  (and symmetry related points), and there are no indications of pair clustering in a compact region (which would correspond to  $q = (\delta, \delta)$ ).

To determine the presence of a superconducting phase, considering the hard core bosons as tightly-bound Cooper

pairs, we compute the equal-time current-current correlations:

$$C_{\alpha\alpha}(\mathbf{r}) = \frac{1}{N} \sum_i \langle j_\alpha(i) j_\alpha(i + \mathbf{r}) \rangle \quad (2)$$

where the current operator along direction  $\alpha$  ( $\alpha = \hat{x}, \hat{y}$ ) is:

$$j_\alpha(i) = it \sum_s (b_{i+\alpha}^\dagger c_{i+\alpha,s} c_{i,s}^\dagger b_i - h.c.) \quad (3)$$

We adopt as the SC order parameter the correlation between the total current crossing a border and the current on a reference bond at the maximum distance:

$$\chi_{SC} = \sum_x C_{\hat{y}\hat{y}}(x, L/2) \quad (4)$$

The signs of  $C_{\hat{y}\hat{y}}(\mathbf{r})$  ( $\hat{y}$  is the vertical direction) are shown in Fig. 5. At the maximum  $\chi_{SC}$  (Fig. 5(a)), the pattern shows the presence of current lines extended over all the cluster, while for  $\chi_{SC} \approx 0$ ,  $x \approx 0.5$  (Fig. 5(b)), the current loops are of the size of a single plaquette.

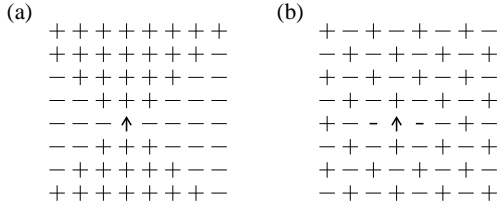


FIG. 5. Signs of  $C_{\hat{y}\hat{y}}(\mathbf{r})$  ( $\hat{y}$  is the vertical direction), (a) at the maximum  $\chi_{SC}$  and (b) for  $\chi_{SC} \approx 0$ ,  $x \approx 0.5$ . The arrows indicate the reference bond

The most important results obtained with the present model concern the superconducting order parameter shown in Fig. 6.  $\chi_{SC}$  and  $C_{\hat{y}\hat{y}}(\mathbf{r})$  at the maximum distance along  $\hat{y}$  have a similar behavior. Even though there are important error bars, there are two apparent qualitative features. In the first place as  $\Lambda$  is reduced ( $\Lambda = 8$  is representative of the  $\Lambda \rightarrow \infty$  behavior) the onset of the SC phase is pushed to higher values of pair density. This feature may be a consequence of AF order at larger densities although, as said before, a finite size extrapolation should be done to determine the phase boundaries. Second, the intensity of  $\chi_{SC}$  is reduced as  $\Lambda$  decreases, i.e. as more  $S^z = \pm 1$  sites are present in the system. In other words, there is a maximal SC signal in the hard-core boson model and this signal is reduced as the isotropic spin-1 model is approached.

It is also instructive to compare the behavior of  $\chi_{SC}$  with the one of the kinetic energy per site shown in Fig. 4(b). Both  $\chi_{SC}$  and  $\langle K \rangle / N$  decrease with  $\Lambda$  for a given  $x$ , although this effect is more intense in the former quantity. The suppression of both quantities near

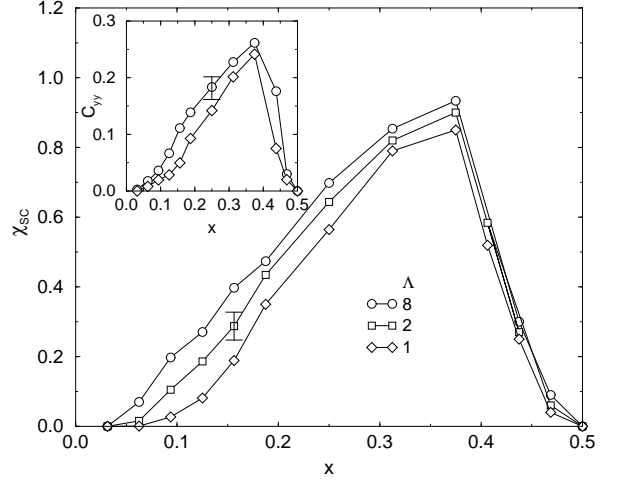


FIG. 6. Superconducting order parameter  $\chi_{SC}$  as a function of pair density and for several values of  $\Lambda$ . The current-current correlations  $C_{\hat{y}\hat{y}}$  at the maximum distance along  $\hat{y}$  are shown in the inset as a function of pair density and for  $\Lambda = 1$  and 8. Typical error bars are shown.

$x = 0.5$  may be due to the charge localization in the  $(\pi, \pi)$  solid phase. Actually, since  $\chi_{SC}$  and  $C(\pi, \pi)$  are sizable for  $x \geq 0.4$ , this suggests a coexistence of SC and the checkerboard solid in this region, which corresponds to the PS region found above.<sup>13</sup> On the other hand, the suppression of SC at low densities has no counterpart in the behavior of the kinetic energy. The characteristics of this region are hence indicating the presence of a AF Mott insulating phase.

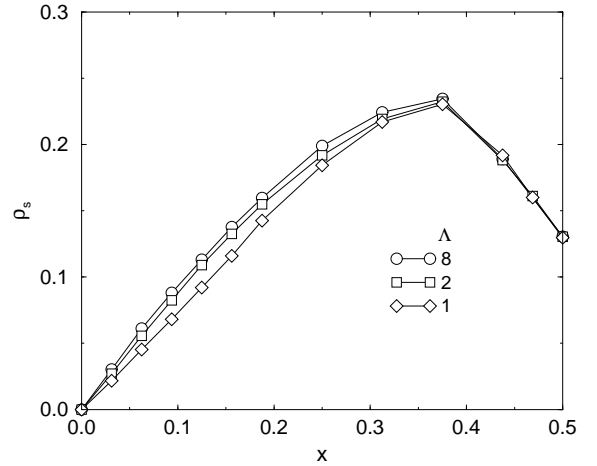


FIG. 7. Superfluid density as a function of pair density and for several values of  $\Lambda$ .

Finally in Fig. 7 we show the superfluid density which is a quantity more conventionally studied in the context of hard-core bosons. This quantity is computed as<sup>15</sup>

$$\rho_s = \int_0^\beta \langle j_\alpha(\tau) j_\alpha \rangle d\tau \quad (5)$$

where  $\tau$  is the imaginary time,  $\beta = 1/T$  and  $j_\alpha(\tau) = \sum_i j_\alpha(i, \tau)$ . As it can be seen in this Figure,  $\rho_s$  has the same qualitative behavior as the kinetic energy per site. Hence, as discussed above, it differs with  $\chi_{SC}$  in the behavior at low pair density.

In summary, a model of pairs as hard-core bosons interacting with spin-1 sites has been proposed to study the interplay between superconductivity and antiferromagnetism. Using quantum Monte Carlo techniques, its main features as a function of pair density and single-ion anisotropy have been determined. Even in this “toy” model some features, which could have some relevance to high- $T_c$  superconductivity, have been observed. The most important feature is the suppression of superconductivity, as long range coherence of preformed pairs, due to the presence of both antiferromagnetism and  $S^z = \pm 1$  excitations, which in this model represent triplet excitations in more realistic models. Indications of incommensurate charge ordering and phase separation have also been observed. This model certainly deserves further investigation. In particular, the dynamical correlations between doublets and pairs should be examined. Finally, the proposed model is relatively simple and hence it can be expected to describe other physical systems. In fact, the model can describe a variety of spin-1 systems with a layered structure like  $\text{La}_{2-x}\text{Sr}_x\text{NiO}_4$  (Ref. 16) or with two-dimensionally coupled chains.<sup>17</sup> Hole pairs could appear in the former compound if there is an on-site attraction present.

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<sup>14</sup> A number of models interpolating between the  $t$ - $J$  model and the present one, and including details like dimer orientation, can be found in the literature. See e.g. Refs. 6,8; Ehud Altman and Assa Auerbach, *cond-mat/0108087*.

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